alpha-d-glucopyranose 492-62-6 | DTXSID30197710

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 2.66 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.79e-01

Confidence level: 5.65e-01

Nearest Neighbors from the Training Set

Image not found

D-Glucose

Measured: 4.08 Predicted: 2.66

Image not found

Galactose

Measured: 4.08 Predicted: 2.66

Image not found

alpha-d-glucopyranose

Measured: 4.08 Predicted: 2.66

Image not found

D-Mannose Measured: 4.08 Predicted: 2.66 Image not found

Anhydromethylenecitric acid

Measured: 2.45e-01 Predicted: 2.45e-01 Image not found

Meglumine
Measured: 3.62
Predicted: 2.83

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Chelidonic acid
Measured: 7.77e-02
Predicted: 1.22e-01

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Pantothenic acid Measured: 4.56 Predicted: 2.37